

Quantum Isomorphic Simulation

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ABSTRACT

A new type of quantum simulator is proposed which can simulate any quantum many-body system in an isomorphic manner. It can actually synthesize a duplicate of the system to be simulated. The isomorphic simulation has the great advantage that the inevitable coupling of the simulator to the environment can be fully exploited in simulating thermodynamic processes.

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Simulating quantum many-body systems on a classical computer is hard in the sense that the simulation takes exponentially long time and large memory as the size of the system increases [1,2]. The difficulty stems from the fact that the Hilbert space of the system consists of exponentially many states as the function of the number of physical variables involved. The efficiency of simulating a system by another well controlled quantum system (quantum computer) was conjectured by Feynman [1] and has been justified by Lloyd [2]. Because of the decoherence problem [3], despite the recent advancement of the quantum computation theory especially on quantum error correction [4,5], it remains to see whether one can construct a large size quantum computer and maintain the delicate quantum coherence in order to accomplish meaningful computations or simulations, although many efforts have been made to implement quantum gates or small size quantum computers [6].

Here we propose that a universal quantum isomorphic simulator (IS) can be constructed by tailoring the many-body interactions among a suitable physical system. Just for convenience in this paper, the system being simulated is called the simulatee. One may choose physical systems consisting of, for example, many isolated quantum wires each with a freely moving electron inside,

or isolated one-dimensional arrays of Josephson junctions [7] each having a magnetic fluxon freely moving back and forth. The position of the electron in the wire or the fluxon in the Josephson junction array provides one continuous degree of freedom which can be assigned to a continuous variable of the simulatee. For simplicity, we will use the terms *wire* and *particle* in the following, whether they are a quantum wire and an electron or a Josephson junction array and a fluxon. Given the Hamiltonian

$$H(t) = H_0 + H'(t),$$

where H_0 describes the unperturbed system of simulatee and $H'(t)$ is the external perturbation, one can tailor the many-body interactions among the system of wires which is called a quantum isomorphic simulator such that the Hamiltonian describing the simulator is identical (in some sense) to $H(t)$, the Hamiltonian of the simulatee. This is why it is called an isomorphic simulator. First note that $H_0 - K$ can be decomposed into a sum of two-body interactions in general, $H_0 - K = \sum_{ij} h_{ij}(x_i, x_j)$, where x_i, x_j are continuous variables which can be simulated by two wires (of course, discrete variables can also be simulated using wires with double potential wells or something else), and the external perturbation $H'(t)$ is a sum of one-body potentials, $H'(t) = \sum_k g_k(x_k)$, K is the total kinetic energy of the simulatee which is naturally mimicked by the inherent inertial motion of the particles (electrons or fluxons) of the simulator. One may divide each wire into N parts (discretization with precision $1/N$), the position-dependent interaction $h_{ij}(x_i, x_j)$ between two wires can be achieved by drawing N^2 connections between the two wires so that the interaction potential of the i th particle at position x_i and the j th particle at position x_j is proportional to $h_{ij}(x_i, x_j)$. For example, if the wires are Josephson junction arrays and the particles are magnetic fluxons, one may enclose the magnetic fluxes at each pair of discrete positions (x_i, x_j) by a superconducting

ring so that the subsystem of the ring and the i th and j th fluxons has a total interaction energy $h_{ij}(x_i, x_j)$ when the i th fluxon is at position x_i and the j th fluxon is at x_j [8-10]. The one-body potentials $g_k(x_k)$ can be easily realized by applying position-dependent external fields to the particles. A simulatee with M continuous variables can be simulated by an IS consisting of M wires, at most $\frac{1}{2}M(M-1)N^2$ connections and no more than MN externally applied fields, with $1/N$ discretization precision. The cost of physical resources is polynomially bounded, and the simulator simulates the simulatee in an isomorphic manner, *i.e.* there is one-to-one correspondence between the essential Hilbert spaces of the two systems, with the eigenenergies of two corresponding states proportional to each other; the two systems are governed by the same Hamiltonian (up to a proportion factor) and undergo the identical dynamics up to a proportion factor in energy and time *etc.*

To understand more about what isomorphic means, one may compare the IS with the conventional (quantum) simulator (CS) [2]. On a CS, there is generally no one-to-one correspondence between the eigenstates of the simulator and the simulatee with the corresponding energies proportional to each other. In particular, the ground state of the simulatee is represented by the ground state of the IS, while the lowest energy state of the CS can not encode the ground state of the simulatee because that ground state is not known *a priori*. Although a CS may exploit the inevitable coupling with the environment to simulate open systems [2], the exploitation is strictly limited. For example, when simulating the relaxation process of an excited system, a CS should at least preserve some energy to encode the information for the ground state of the simulatee. These remaining excitations make the system unstable and vulnerable to perturbations. By contrast, an IS is not so niggardly, it happily dissipates all its energy and gets to the lowest energy level which represents the ground state of the simulatee. This example has already demonstrated one scheme for an IS to simulate thermodynamic processes. Since the IS is just a duplicate of the simulatee in the isomorphic sense, its natural relaxation naturally mimics the relaxation of the simulatee. This scheme is particularly useful to simu-

late these relaxation processes where the actual forms of the external perturbations are subordinate, what really important are the internal structure of the simulatee and the statistics of the perturbations. To this extent, an IS is outstanding in simulating the thermodynamics and dynamics of complex systems such as biological macromolecules [11] and atomic and molecular clusters [12]. With a proper Hamiltonian describing the interactions among smaller pieces of the complex system and some random terms mimicking the stochastic perturbations, a classical computer may provide some information, but a full simulation takes exceedingly long time. By contrast, if provided with the correct Hamiltonian, an IS can synthesize a duplicate of the complex system, the motion of the duplicate is identical to the simulatee in the isomorphic sense that there is one-to-one correspondence between the eigenstates and the corresponding energies are proportional to each other, the dynamics of the two systems are identical up to a constant factor in time scale. For instance, if provided with the correct Hamiltonian describing the interactions among the amino acids and their interactions with water, a synthesized *protein* on an IS should *fold* itself very fast as the real protein does [11]. On an IS, scientists can test their models and design new complex systems conveniently. To simulate dynamic processes with well-defined driving forces on an IS, dissipation should be avoided and one needs to apply external fields with proper forms to simulate the real driving forces.

In conclusion, the proposed quantum simulator can simulate any quantum many-body system in an isomorphic manner. The cost of physical resources is bounded by a polynomial function of the size of the system to be simulated and the simulation takes a time proportional to the time of the real process. The great advantage of the isomorphic simulation is that there is a one-to-one correspondence between the eigenstates of the simulator and the simulatee, the corresponding energies are proportional to each other, the two systems are governed by the same equation of motion. In particular, the ground state of the simulator corresponds to the ground state of the simulatee. Consequently, an IS is outstanding in simulating natural thermodynamic phenomena. The inevitable perturbations from the en-

vironment can be fully and naturally exploited when simulating real thermodynamic processes. At present the well-established technology for superconductive devices is very promising to implement an IS using Josephson junction arrays [8-10]. The continuing advancement in fabricating small size devices may eventually make it possible to implement IS' in terms of semiconductor nanostructures [13]. It is exciting to expect that in the near future quantum isomorphic simulators are widely used to synthesize and test various complex systems.

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